C51	0.1350 (5)	0.4455 (4)	0.0350 (9)	0.062 (2)
C61	0.2241 (5)	0.3581 (4)	−0.2420 (7)	0.065 (2)
B1	0.3064 (6)	0.2731 (8)	0.3236 (9)	0.066 (2)
B3	0.3649 (6)	0.3346 (6)	0.1754 (10)	0.059 (2)
B4	0.4415 (7)	0.2786 (9)	0.3228 (11)	0.078 (3)

Table 2. *Selected geometric parameters* (Å, °)

Ru2—C6	2.189 (5)	Ru2—B3	2.370 (8)
Ru2—C5	2.201 (5)	Ru2—B1	2.379 (8)
Ru2—C4	2.200 (5)	Ru2—Cl	2.391 (2)
Ru2—C3	2.207 (5)	B1—B3	1.725 (12)
Ru2—C1	2.220 (6)	B1—B4	1.812 (12)
Ru2—C2	2.224 (5)	B3—B4	1.810 (12)
B3—Ru2—B1	42.6 (3)	B4—B1—Ru2	110.3 (5)
B3—Ru2—Cl	92.9 (2)	B1—B3—B4	61.6 (5)
B1—Ru2—Cl	96.2 (2)	B1—B3—Ru2	69.0 (4)
B3—B1—B4	61.5 (5)	B4—B3—Ru2	110.8 (5)
B3—B1—Ru2	68.4 (4)	B3—B4—B1	56.9 (5)

Hexamethylbenzene H atoms were placed in calculated positions riding on the C atoms to which they are bonded. Borane H atoms were located on difference maps and their parameters refined. All H atoms were given isotropic displacement parameters of 0.1 $Å^2$.

Data collection: CAD-4 software. Cell refinement: CAD-4 software. Data reduction: *SDP-Plus* (Enraf–Nonius, 1985). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEP* (Johnson, 1965).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1106). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Aqua(1,10-phenanthroline)(L-serinato)-copper(II) Nitrate

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Abstract

The unit cell of the title complex, $[Cu(C_3H_6NO_3)(C_{12}H_8N_2)(H_2O)]NO_3$, contains two nitrate anions and two complex cations, each with two chiral centers, one in the serine molecule and the other at the Cu ion. Each Cu ion displays slightly distorted square-pyramidal coordination, with the water molecule in the apical position and the base defined by the aliphatic N atom and one of the O atoms from the aminocarboxylate ligand and the two N atoms from the phenanthroline molecule. The relative position of the apical water molecule generates the chiral center at the Cu ion. In both molecules, the five-membered chelate ring defined by atoms N1, C12, C11, N2 and Cu is roughly planar, while the ring defined by atoms N3, C13, C14, O1 and Cu has a distorted half-chair conformation.

Comment

Our study of the anticancer properties of several mixed phenanthroline–aminocarboxylate complexes led us to prepare and crystallize the complex $[Cu(H_2O)$(L-ser)(phen)$]NO_3$ (L-ser is L-serine and phen is 1,10-

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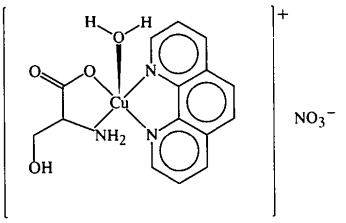
phenanthroline), (I), as reported elsewere (Gasque, Ruiz-Ramírez, & Moreno-Esparza, 1992), in order to obtain a more detailed understanding of this type of complex.



(I)

A view of one of the stereoisomers of $[Cu(H_2O)$(L-ser)(phen)$]NO_3$, together with the atom numbering, is shown in Fig. 1. The other molecule (not shown) is correspondingly labeled with primes. A view of the contents of the unit cell is shown in Fig. 2. It contains two complex cations, each with two chiral centers, one in the serine ligand and the other at the Cu ion.

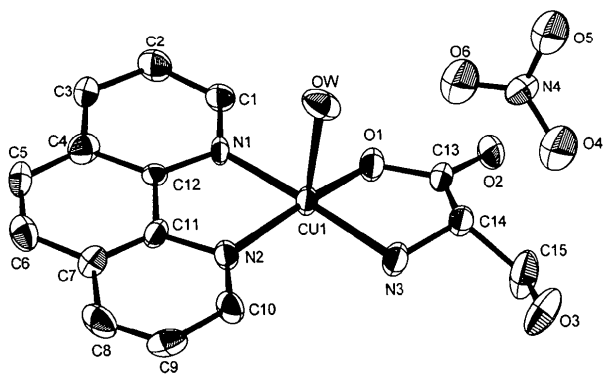


Fig. 1. *ORTEP* plot (*PC-ORTEP*; Schmid & Bruggemann, 1990*a*) of the molecular structure of $[Cu(H_2O)$(L-ser)(phen)$]NO_3$. Non-H atoms are represented by their 50% probability displacement ellipsoids and H atoms are omitted.

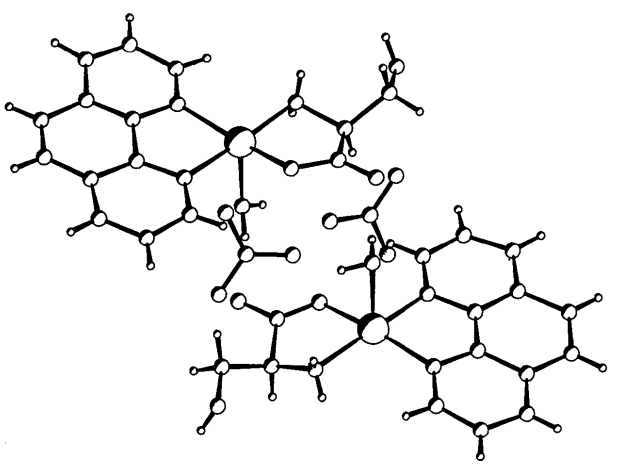


Fig. 2. *PLUTO* view (*PC-PLUTO*; Schmid & Bruggemann, 1990*b*) of the unit cell showing both stereoisomers.

The relative position of the apical water molecule with respect to the serine moiety generates the chiral center at each Cu ion.

Each Cu ion is surrounded by five ligand atoms in a slightly distorted square-pyramidal configuration, where the water molecule is in the apical position and the base is defined, with negligible tetrahedral distortion, by the aliphatic N atom and one of the O atoms from the carboxylate ligand and the two N atoms from the phenanthroline ligand. The distances to the least-squares plane defined by atoms N1, N2, N3 and O1 in one of the stereoisomers are N1 −0.065 (3), N2 0.060 (3), N3 −0.060 (3) and O1 −0.066 (3) Å, while for the plane defined by atoms N1′, N2′, N3′ and O1′ the deviations are N1′ 0.068 (3), N2′ −0.062 (3), N3′ 0.062 (3) and O1′ −0.069 (3) Å. The Cu1 and Cu2 ions are 0.194 (3) and 0.194 (3) Å, respectively, out of their respective least-squares mean coordination planes.

Other relevant mean planes are the five-membered phenanthroline chelate rings, defined by atoms N1, C12, C11, N2 and Cu1, and N1′, C12′, C11′, N2′ and Cu2, which are roughly planar [the average r.m.s. deviation from five fitted atoms is 0.097 (1) Å, for both stereoisomers], while the ring defined by atoms N3, C13, C14, O1 and Cu1, and that defined by N3′, C13′, C14′, O1′ and Cu2, deviate significantly from planarity, presenting a distorted half-chair conformation in each case.

The angles between the least-squares mean planes of the phenanthroline molecules and the aminocarboxylate chelation rings are 5.1 (3) and 12.5 (3)° for the Cu1 and Cu2 complexes, respectively. On the other hand, the angle between the basal coordination mean plane and the phenanthroline ligand is 9.1 (2)° for the Cu1 complex and 7.8 (2)° for the Cu2 complex, while the angles formed with the aminocarboxylate chelation ring are 8.9 (2) and 17.1 (3)° for the Cu1 and Cu2 complexes, respectively.

The average Cu—N distance [2.010 (10) Å] is longer than the Cu—O1 distance [1.935 (3) Å], as observed in many related complexes (Aoki & Yamasaky, 1980; Antolini, Marcotrigiano, Menabue & Pellacani, 1983; Antolini, Marcotrigiano, Menabue, Pellacani, Saladini & Sola, 1985; Antolini, Battaglia, Corradi, Marcotrigiano, Menabue, Pellacani, Saladini & Sola, 1986; Mendoza-Diaz, Martínez-Aguilera, Pérez-Alonso, Solans & Moreno-Esparza, 1987; Solans, Ruiz-Ramírez, Martínez, Gasque & Briansó, 1988; Solans, Ruiz-Ramírez, Martínez, Gasque & Moreno-Esparza, 1992, 1993; Mendoza-Diaz, Martínez-Aguilera, Moreno-Esparza, Pannell & Cervantes Lee, 1993).

The Cu—O(aqua) bond length is similar to those observed in other related complexes; 2.275 (3) Å for both molecules in this compound, 2.294 (6) Å for the L-glutamate complex (Antolini, Marcotrigiano, Menabue, Pellacani, Saladini & Sola, 1985; Antolini, Battaglia, Corradi, Marcotrigiano, Menabue, Pellacani, Saladini &

Sola, 1986) and 2.213 (10) Å for the L-phenylalaninato complex (Solans, Ruiz-Ramírez, Martínez, Gasque & Briansó, 1988).

The nitrate ion is not involved in the coordination sphere of the Cu ion and the nearest neighbour (O6) is as far as 4.9 Å away. The asymmetric unit is stabilized by hydrogen bonding: *OW*—H1*W*···O2′ [H···O 1.94, O···O 2.76 Å], *OW*—H1*W*···O6 [H···O 2.04, O···O 2.83 Å], *OW′*—H3*W*···O2 [H···O 1.83, O···O 2.68 Å]. Crystal packing is determined by weak hydrogen bonding and probably also by π–π^* interactions between phenanthroline units.

Experimental

Suitable crystals for X-ray analysis were grown by slow evaporation from a water solution.

Crystal data

$[Cu(C_3H_6NO_3)(C_{12}H_8N_2)(H_2O)]NO_3$
M_r = 427.86
Triclinic
$P\bar{1}$
a = 7.624 (2) Å
b = 10.027 (2) Å
c = 12.001 (3) Å
α = 97.46 (1)°
β = 106.79 (1)°
γ = 108.76 (1)°
V = 806.2 (3) Å^3
Z = 2
D_x = 1.763 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 11.470–24.402°
μ = 1.406 mm^{-1}
T = 294 (2) K
Prismatic
0.55 × 0.33 × 0.20 mm
Blue

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scans using 9 reflections
T_{min} = 0.9318, T_{max} = 0.9999
5087 measured reflections
5087 independent reflections
4355 observed reflections [$I > 2\sigma(I)$]
θ_{max} = 30.40°
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = 0 \rightarrow 17$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.0383
$wR(F^2)$ = 0.1070
S = 1.046
5087 reflections
485 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0560P)^2 + 0.7766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.495
$\Delta\rho_{max}$ = 1.139 e Å^{-3}
$\Delta\rho_{min}$ = −0.810 e Å^{-3}
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983); χ = 0.06 (2)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Cu1	0.46104 (6)	0.67527 (5)	0.86369 (4)	0.0266 (2)
N1	0.7002 (5)	0.8473 (4)	0.9733 (3)	0.0234 (13)
N2	0.5121 (7)	0.5943 (5)	1.0111 (3)	0.0272 (14)
N3	0.2014 (5)	0.5221 (5)	0.7577 (4)	0.038 (2)
OW	0.6490 (7)	0.5895 (5)	0.7808 (4)	0.0438 (15)
O1	0.3982 (7)	0.7905 (4)	0.7522 (3)	0.0354 (13)
O2	0.2056 (8)	0.7687 (7)	0.5655 (5)	0.0380 (12)
O3	−0.1532 (9)	0.3526 (7)	0.5592 (7)	0.052 (2)
C1	0.7896 (12)	0.9702 (8)	0.9487 (7)	0.030 (2)
C2	0.9598 (13)	1.0802 (9)	1.0331 (7)	0.037 (2)
C3	1.0347 (11)	1.0630 (9)	1.1494 (6)	0.030 (2)
C4	0.9442 (12)	0.9329 (9)	1.1796 (8)	0.033 (2)
C5	1.0018 (12)	0.9037 (9)	1.2897 (7)	0.0329 (5)
C6	0.9030 (13)	0.7766 (9)	1.3091 (7)	0.036 (2)
C7	0.7355 (10)	0.6665 (8)	1.2175 (7)	0.029 (2)
C8	0.6223 (15)	0.5354 (11)	1.2347 (8)	0.042 (2)
C9	0.4676 (12)	0.4361 (9)	1.1415 (8)	0.037 (2)
C10	0.4185 (11)	0.4725 (9)	1.0294 (6)	0.030 (2)
C11	0.6717 (10)	0.6913 (8)	1.1088 (6)	0.027 (2)
C12	0.7735 (10)	0.8301 (7)	1.0833 (6)	0.0208 (13)
C13	0.2545 (10)	0.7164 (8)	0.6512 (6)	0.0269 (13)
C14	0.1524 (6)	0.5541 (5)	0.6388 (4)	0.0273 (8)
C15	−0.0659 (14)	0.5021 (11)	0.5737 (8)	0.055 (2)
Cu2	0.64688 (6)	0.92114 (5)	0.45344 (4)	0.0271 (2)
N1′	0.4101 (6)	0.7478 (4)	0.3434 (4)	0.0267 (13)
N2′	0.5968 (7)	0.9997 (5)	0.3049 (3)	0.0249 (13)
N3′	0.9048 (6)	1.0762 (4)	0.5601 (4)	0.036 (2)
OW′	0.4553 (7)	1.0061 (6)	0.5335 (5)	0.047 (2)
O1′	0.7110 (7)	0.8077 (4)	0.5666 (4)	0.040 (2)
O2′	0.9217 (8)	0.8167 (6)	0.7381 (5)	0.0379 (12)
O3′	1.2619 (10)	1.2478 (8)	0.7606 (8)	0.058 (2)
C1′	0.3201 (12)	0.6233 (9)	0.3673 (7)	0.030 (2)
C2′	0.1528 (10)	0.5127 (8)	0.2809 (7)	0.033 (2)
C3′	0.0772 (12)	0.5307 (9)	0.1716 (8)	0.039 (2)
C4′	0.1715 (10)	0.6625 (8)	0.1441 (6)	0.0227 (13)
C5′	0.1013 (12)	0.6944 (9)	0.0245 (7)	0.0329 (5)
C6′	0.2044 (11)	0.8221 (9)	0.0029 (6)	0.030 (2)
C7′	0.3781 (11)	0.9305 (9)	0.0962 (6)	0.0265 (15)
C8′	0.4865 (11)	1.0663 (8)	0.0826 (7)	0.0290 (15)
C9′	0.6488 (12)	1.1634 (9)	0.1795 (7)	0.035 (2)
C10′	0.6982 (11)	1.1295 (8)	0.2893 (8)	0.035 (2)
C11′	0.4395 (10)	0.9020 (8)	0.2139 (6)	0.0208 (13)
C12′	0.3370 (11)	0.7698 (9)	0.2313 (6)	0.0254 (15)
C13′	0.8698 (11)	0.8663 (8)	0.6517 (6)	0.0285 (13)
C14′	1.0162 (6)	1.0072 (5)	0.6430 (4)	0.0281 (8)
C15′	1.1480 (15)	1.1090 (11)	0.7635 (9)	0.055 (2)
N4	0.3525 (6)	0.3080 (6)	0.4571 (5)	0.0351 (14)
O4	0.1715 (7)	0.2542 (9)	0.4336 (6)	0.0723 (11)
O5	0.4228 (9)	0.2837 (8)	0.3797 (5)	0.0723 (11)
O6	0.4689 (8)	0.3985 (7)	0.5501 (5)	0.0723 (11)
N4′	0.7487 (8)	0.2865 (8)	0.8542 (5)	0.056 (2)
O4′	0.9305 (7)	0.3349 (10)	0.8794 (6)	0.0745 (11)
O5′	0.6799 (9)	0.2889 (8)	0.9354 (6)	0.0745 (11)
O6′	0.6301 (8)	0.2551 (7)	0.7515 (5)	0.0745 (11)

Table 2. *Selected geometric parameters* (Å, °)

Cu1—O1	1.934 (2)	Cu2—O1′	1.937 (2)
Cu1—N3	1.994 (3)	Cu2—N3′	1.996 (3)
Cu1—N1	2.008 (2)	Cu2—N1′	2.008 (2)
Cu1—N2	2.029 (2)	Cu2—N2′	2.026 (2)
Cu1—*OW*	2.275 (3)	Cu2—*OW′*	2.275 (3)
N1—C1	1.320 (8)	N1′—C1′	1.329 (9)
N1—C12	1.334 (8)	N1′—C12′	1.376 (9)
N2—C10	1.284 (9)	N2′—C11′	1.342 (9)
N2—C11	1.386 (8)	N2′—C10′	1.352 (8)
N3—C14	1.472 (7)	N3′—C14′	1.503 (6)
O1—C13	1.303 (8)	O1′—C13′	1.236 (8)
O2—C13	1.232 (9)	O2′—C13′	1.226 (9)
O3—C15	1.394 (12)	O3′—C15′	1.395 (12)
C1—C2	1.399 (11)	C1′—C2′	1.400 (10)

C2—C3	1.404 (10)	C2′—C3′	1.333 (12)
C3—C4	1.413 (11)	C3′—C4′	1.419 (12)
C4—C5	1.368 (12)	C4′—C12′	1.384 (10)
C4—C12	1.432 (11)	C4′—C5′	1.495 (10)
C5—C6	1.344 (12)	C5′—C6′	1.372 (12)
C6—C7	1.423 (11)	C6′—C7′	1.446 (10)
C7—C11	1.341 (11)	C7′—C8′	1.406 (11)
C7—C8	1.400 (12)	C7′—C11′	1.451 (9)
C8—C9	1.351 (13)	C8′—C9′	1.389 (10)
C9—C10	1.418 (10)	C9′—C10′	1.381 (11)
C11—C12	1.478 (10)	C11′—C12′	1.382 (11)
C13—C14	1.527 (8)	C13′—C14′	1.531 (8)
C14—C15	1.496 (10)	C14′—C15′	1.503 (10)
O1—Cu1—N3	84.7 (2)	O1′—Cu2—N3′	84.5 (2)
O1—Cu1—N1	90.9 (2)	O1′—Cu2—N1′	91.2 (2)
N3—Cu1—N1	171.7 (2)	N3′—Cu2—N1′	171.8 (2)
O1—Cu1—N2	163.9 (2)	O1′—Cu2—N2′	163.6 (2)
N3—Cu1—N2	100.3 (2)	N3′—Cu2—N2′	100.4 (2)
N1—Cu1—N2	82.1 (2)	N1′—Cu2—N2′	81.9 (2)
O1—Cu1—*OW*	97.8 (2)	O1′—Cu2—*OW*′	98.1 (2)
N3—Cu1—*OW*	96.0 (2)	N3′—Cu2—*OW*′	95.9 (2)
N1—Cu1—*OW*	91.5 (2)	N1′—Cu2—*OW*′	91.6 (2)
N2—Cu1—*OW*	96.8 (2)	N2′—Cu2—*OW*′	96.9 (2)
N1—C12—C11—N2	1.4 (9)	O1—C13—C14—N3	16.1 (7)
N1′—C12′—C11′—N2′	−1.4 (9)	O1′—C13′—C14′—N3′	23.8 (8)

H atoms bonded to C atoms were positioned geometrically and refined with a common U value. The remaining H atoms were located by difference Fourier synthesis and refined using distance restraints and common U values.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software* (Enraf–Nonius, 1989). Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PC-ORTEP* (Schmid & Brueggemann, 1990*a*) and *PC-PLUTO* (Schmid & Brueggemann, 1990*b*).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1141). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Disilver *cis*-Butenedioate

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Abstract

Disilver *cis*-butenedioate, $[Ag_2(C_4H_2O_4)]$, has been synthesized and compared with other Ag carboxylates. One of the Ag atoms coordinates to the C=C double bond in the *cis*-butenedioic acid (trivial name: maleic acid) at a distance of 2.40 (1) Å.

Comment

Several Ag^I carboxylate complexes have hitherto been characterized by X-ray diffraction methods (Chen & Mak, 1991*a*,*b*). Some salient features of these compounds are (*a*) the aggregation of Ag atoms in dimers or, less commonly, polymers, and (*b*) the bridging carboxylate group connecting the metal atoms in the dimer.

The title compound, (I), can be characterized as containing isolated silver dimers. However, the Ag···Ag distance is significantly longer than the metal–metal contacts found in other dimeric silver(I) carboxylates, indicating a weak Ag···Ag interaction in the present compound. Moreover, no conclusion about bonding interactions can be drawn exlusively from the metal–metal distance (Jansen, 1987). The next shortest Ag···Ag contact is within the van der Waals radius of Ag, 3.44 Å (Bondi 1964). If this elongated Ag···Ag contact is in-

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